

README created on 2023-11-03 by Xiaojia Wang

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GENERAL INFORMATION  
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Title of Dataset:

Supporting Data for Temperature-dependent Thermal Conductivity of MBE-Grown Epitaxial SrSnO<sub>3</sub> Films

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Date of data collection: 20211214 - 20230629

Geographic location of data collection: University of Minnesota

Information about funding sources that supported the collection of the data:

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SHARING/ACCESS INFORMATION  
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Recommended citation for the data: Zhang, Chi; Liu, Fengdeng; Guo, Silu; Zhang, Yingying; Xu, Xiaotian; Mkhoyan, Andre; Jalan, Bharat; Wang, Xiaojia. (2023). Supporting data for Temperature-dependent thermal conductivity of MBE-grown epitaxial SrSnO<sub>3</sub> films. Retrieved from the Data Repository for the University of Minnesota, <https://doi.org/10.13020/tmn3-ds92>.

1. Licenses/restrictions placed on the data: [CC0 1.0 Universal](#)
2. Links to publications that cite or use the data: Chi Zhang, Fengdeng Liu, Silu Guo, Yingying Zhang, Xiaotian Xu, K. Andre Mkhoyan, Bharat Jalan, Xiaojia Wang; Temperature-dependent thermal conductivity of MBE-grown epitaxial SrSnO<sub>3</sub> films. Appl. Phys. Lett. 24 July 2023; 123 (4): 042201. <https://doi.org/10.1063/5.0156367>
3. Links to other publicly accessible locations of the data: NA
4. Links/relationships to ancillary data sets: NA
5. Was data derived from another source? No

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DATA & FILE OVERVIEW  
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1. File List

A. Filename: SSO\_source\_AllData\_11\_02\_2023.xlsx

Short description: One excel containing all raw data for plots, including the main paper and the Supplementary Material, following the order of figure numbers.

B. Filename: AllData\_Archive.zip

Short description: Raw data for plots, including the main paper and the Supplementary Material, following the order of figure numbers (same as SSO\_source\_AllData\_11\_02\_2023 but converted to 11 .csv).

2. Relationship between files: Same data, different formats
3. Additional related data collected that was not included in the current data package: No

4. Are there multiple versions of the dataset? No

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METHODOLOGICAL INFORMATION  
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1. Description of methods used for collection/generation of data:

**Sample synthesis with the hybrid molecular beam epitaxy (MBE)**

The hybrid MBE approach for SSO synthesis employs a conventional solid source for Sr, hexamethylditin (HMDT) as a metal-organic precursor for Sn, and an inductively coupled RF plasma for O. The Sr beam equivalent pressure (BEP, *a.k.a.*, the pressure exerted on the substrate by the Sr gas beam), measured with a beam flux monitor, was fixed at  $6 \times 10^{-8}$  Torr. The BEP ratio of HMDT and Sr was kept at 400 to ensure stoichiometric films. The oxygen flow was set to 0.7 sccm to achieve an oxygen background pressure of  $5 \times 10^{-6}$  Torr while applying an RF power of 250 W to the plasma coil. The calibrated deposition rate is  $31 \text{ nm h}^{-1}$  under these growth conditions. The thin film was grown on a SrTiO<sub>3</sub> substrate at 950 °C for 10 hrs.

**Structural Characterization with scanning transmission electron microscopy (STEM)**

The cross-sectional lamellas for STEM study were prepared using Focused Ion Beam (FEI Helios NanoLab G4 dual-beam). A protection layer of 2 μm amorphous C was deposited on the region of interest prior to ion beam trenching. Focused ion beam (FIB) was operated at 30 kV. STEM experiments were carried out on an aberration-corrected FEI Titan G2 60–300 (S)TEM microscope equipped with a CEOS DCOR probe corrector, monochromator, and a super-X energy dispersive X-ray (EDX) spectrometer. STEM was operated at 200 kV for all measurements. HAADF-STEM images were obtained with a probe current of 50 pA. Camera length was set to be 130 mm with a probe convergence angle of 25.5 mrad for imaging. The detector inner angle was 55 mrad and outer collection angle was 200 mrad.

**The X-ray diffraction (XRD) rocking curve of the STO substrate**

The thermal conductivities of the bulk STO substrate obtained from TDTR are slightly lower than the literature data at intermediate and high temperatures (150 K and above). To explore the possible explanations for this discrepancy, we conducted XRD rocking curve measurements on the STO substrate along the [001] direction. The appearance of asymmetric peak in the XRD rocking curve (Fig. S1) indicates poor crystalline quality including small-angle tilts, boundaries, and dislocations, leading to a lower thermal conductivity.

**TDTR measurements**

We used TDTR to measure the through-plane thermal conductivity ( $\Lambda_{SSO}$ , along [001]) of the single crystalline SSO film from 90 to 500 K. Prior to TDTR measurements, an aluminum (Al) layer was sputtered onto the sample as a transducer. A reference of 300-nm SiO<sub>2</sub>/Si and a bulk STO substrate were placed next to the sample for transducer preparation, as control samples for thermal measurements. For TDTR measurements, a 5× objective lens with a  $1/e^2$  radius of  $\approx 12$

$\mu\text{m}$  was used to focus both pump and probe beams onto the sample surface. The pump excitation was modulated at two frequencies ( $f = 9$  and  $18$  MHz). Thermal transport in the sample stack is considered as thermal wave propagation at the modulation frequency producing a thermal penetration depth of  $\delta = \sqrt{\Lambda/\pi f C}$  with  $\Lambda$  and  $C$  being the thermal conductivity and volumetric heat capacity of the sample, respectively. For TDTR measurements, the samples were mounted on a temperature-control stage in an environmental chamber. Measurements were first conducted on the STO substrate to obtain its temperature-dependent (T-dependent)  $\Lambda_{\text{STO}}$ , followed by the measurements of the SSO/STO stack. The setting temperature ( $T_{\text{set}}$ ) varied from 90 to 500 K with the lowest temperature being limited by liquid nitrogen as the coolant. The actual temperature of the sample consists of three parts:  $T_{\text{set}}$ , the steady-state temperature rise ( $\Delta T_{\text{ss}}$ ), and per-pulse temperature rise ( $\Delta T_{\text{pp}}$ ). At low temperatures,  $\Delta T_{\text{pp}}$  can impact the sample temperature substantially due to the reduced heat capacity. Therefore, the nominal  $T_{\text{set}}$  is corrected to reflect the actual temperature of the sample accordingly in the data analysis (Section 4 of the SM).

2. Methods for processing the data: MATLAB R2019b and Origin 2023 were used for data processing and figure generation.

3. Instrument- or software-specific information needed to interpret the data: The plots in the main paper and Supplementary Information were prepared by Origin 2023. The crystal structures in Fig. 1(a) were generated by Vesta.

4. Standards and calibration information, if appropriate: All TDTR measurements on the STO and SSO samples were done after the setup was calibrated by  $\text{SiO}_2$  reference sample measurements. In this way, the reliability of the TDTR measurements was ensured.

5. Environmental/experimental conditions: All the experiments were done within the temperature range of  $\sim 90$  to 500 K.

6. Describe any quality-assurance procedures performed on the data: NA

7. People involved with sample collection, processing, analysis and/or submission:  
List people and their role.

B. J. and X.W. originated the research. A. M., B. J., and X.W. supervised the research. C.Z. and Y.Z. carried out the TDTR measurements and analyses under the guidance of X.W. F.L. prepared the SSO samples and performed the XRD characterization under the guidance of B.J. S. G. performed STEM characterization under the guidance of A. M. C. Z. did the Debye-Callaway model simulations under the guidance of X. W. C. Z., F. L., S. G., X. X., A. M., B. J., and X.W. contributed to the writing of the manuscript. All authors discussed the data and provided input on the paper.